

Kinematic relativity of quantum Hamiltonian

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Abstract

It is shown that the well-known relativistic correction of quantum Hamiltonian that is present in textbooks appears after quantization of oversimplified relativistic kinetic energy decomposition. Using the proper expression one obtains the kinetic energy operator which relation with the usual one is consistent with corresponding relation of kinetic energies in special relativity theory. The Schrödinger equation with this operator gives new interesting possibilities for quantum phenomena description.

Kinetic energy operator is the essential element of nonrelativistic quantum Hamiltonian. Namely this operator defines the type of equation. By definition, this operator appears from classical kinetic energy expression $T_0 = p_0^2/2m$, when instead of momentum $p_0 = mv$ corresponding quantum operator

$$\mathbf{p}_0 = -i\hbar\nabla. \quad (1)$$

is applied. Relativistic corrections for kinetic energy operator are needed for minimal modification of this Hamiltonian. The basic is the kinetic energy definition in Special Relativity Theory (SRT):

$$T = mc^2 \sqrt{1 + (p/mc)^2} - mc^2. \quad (2)$$

which expansion in terms of p/mc is

$$T = \frac{p^2}{2m} \sum_{k=0}^{\infty} \frac{(-1)^k}{(k+1)} \binom{2k}{k} \left(\frac{p}{2mc}\right)^{2k} = \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} + \dots \quad (3)$$

(here $\binom{2k}{k}$ denotes the binomial coefficient). The first member of this expansion is defined as nonrelativistic kinetic energy, and the second provides the mentioned correction. Namely this definition is present in quantum mechanics textbooks, beginning with classical, such as [1],[2],[3] and finishing with the modern ones [4],[5] or [6]. The same expansion also appears in Dirac equation transformation to the Schrödinger form, hence it is widely accepted in journals publications, considering the relativistic corrections of different quantum Hamiltonians.

However, this conclusion follows from definition that at SRT kinetic energy expression (2) quantization the operator $-i\hbar\nabla$ corresponds to the momentum p so that the first term of expansion (3) equals the kinetic energy operator, present in Schrödinger equation. This means that instead of the relativistic kinetic energy (2) simplified form

$$mc^2 \sqrt{1 + (p_0/mc)^2} - mc^2 \quad (4)$$

is applied. As a result, the second term of expansion (3) appears with negative sign, defining that the corrected kinetic energy is smaller than the nonrelativistic one. Obviously, this result is far from reality because the corrected value has to be larger than the nonrelativistic ($T > T_0$ at all momentum values, see Eq.(7)). The well known explanation of this improper conclusion sounds like the one given in [4], where the first term of expansion is called as

"The nonrelativistic kinetic energy", and the second as "The first energy correction, due to the relativistic variation of the mass with the velocity". The result obtained following the widely accepted recommendations is problematic also from point of view of relativistic character of momentum and corresponding operator. Nonrelativistic momentum as function of particle velocity is linear at all values of argument. Behavior of relativistic momentum in this situation is completely another - it takes infinite value at $v = c$ and is undefined for larger velocities. Corresponding quantum operator has to have the analogous dependence, however the standard well-known operator's $-i\hbar\nabla$ eigenvalues spectrum is without any signs of relativity.

As follows from the definition, the problem is that the momentum present in (2) is the relativistic momentum $p = \gamma p_0$, where

$$\gamma = 1/\sqrt{1 - (p_0/mc)^2}. \quad (5)$$

SRT kinetic energy expansion, which first term is namely nonrelativistic kinetic energy, can be obtained applying the given above γ and definition, equivalent to (2) but rewritten as

$$T = mc^2 (\gamma - 1). \quad (6)$$

In this case one can easily obtain the following result:

$$T = mc^2 \sum_{k=1}^{\infty} \binom{2k}{k} \left(\frac{p_0}{2mc} \right)^{2k} = \frac{p_0^2}{2m} + \frac{3p_0^4}{8m^3c^2} + \dots \quad (7)$$

Now, the first member of this expansion exactly corresponds the quantum nonrelativistic kinetic energy operator

$$\mathbf{T}_0 = -\frac{\hbar^2}{2m} \nabla^2, \quad (8)$$

while the second

$$\frac{3}{2} \frac{\mathbf{T}_0^2}{mc^2} \quad (9)$$

can be applied for relativistic corrections of Schrödinger equation eigenvalues. Mean value of this operator, equal $3t_0^2/2mc^2$, at $t_0 \ll mc^2/2$ is small in comparison with nonrelativistic kinetic energy t_0 , obtained after Schrödinger equation solution. However, this correction can be remarkable in situation, when particle is loosely bound in deep potential well. In this case the kinetic and also the potential energies are large, but their difference, equal

binding energy of state under consideration, is small enough. Namely such problems are characteristic for strong interaction potentials of microscopic nuclear theory.

However, this correction does not help taking into account the mentioned relativistic momentum and kinetic energy (2) behavior at particle velocity, approaching c .

This feature of SRT can be taken into account after complete quantization of the first term of expansion (3), equal $T_1 = p^2/2m$. Corrected expression for kinetic energy equals

$$T_1 = \gamma^2 \frac{p_0^2}{2m} = \frac{p_0^2/2m}{1 - (p_0/mc)^2} \equiv \frac{T_0}{1 - 2T_0/mc^2}, \quad (10)$$

and corresponding quantum mechanical operator is

$$\mathbf{T}_1 = (1 - 2\mathbf{T}_0/mc^2)^{-1} \mathbf{T}_0. \quad (11)$$

The eigenfunctions of this operator coincide with corresponding eigenfunctions of operator \mathbf{T}_0 , because the commutator of these operators equals zero. However, every eigenfunction corresponds with different eigenvalues of \mathbf{T}_0 and \mathbf{T}_1 . At nonrelativistic kinetic energy, equal t_0 , the corrected eigenvalue of operator \mathbf{T}_1 equals

$$t_1 = t_0 / (1 - 2t_0/mc^2). \quad (12)$$

Due to positive definiteness of operator \mathbf{T}_1 its eigenvalues have to be positive, hence a condition for nonrelativistic eigenvalue $t_0 < mc^2/2$ appears.

Let us investigate the spectrum of this operator for particle in infinitely deep spherically symmetric well. This is the problem of spherical cavity with completely impenetrable walls. The potential inside of well equals zero and outside of well equals infinity. Schrödinger equation for this problem is well known:

$$\mathbf{T}_0 \varphi_{nl\mu}(\mathbf{r}) = e_{nl} \varphi_{nl\mu}(\mathbf{r}). \quad (13)$$

The boundary condition

$$\varphi_{nl\mu}(|\mathbf{r}| = R) \equiv 0, \quad (14)$$

where the radius of well equals R , defines infinite set of this equation solutions. Here $l\mu$ denotes angular momentum and projection quantum numbers, $n = 1, 2, \dots$ is number of bound state with given l .

For corrected operator with the same boundary condition the corresponding equation is

$$(1 - 2\mathbf{T}_0/mc^2)^{-1} \mathbf{T}_0 \varphi_{nl\mu}(\mathbf{r}) = E_{nl} \varphi_{nl\mu}(\mathbf{r}). \quad (15)$$

The eigenfunctions of both equations - (13) and (15) again coincide, the eigenvalues are different:

$$E_{nl} = \frac{e_{nl}}{1 - 2e_{nl}/mc^2}. \quad (16)$$

This relation clearly demonstrates the considered relativistic character of the corrected problem. As mentioned, kinetic energy operator is positively defined, hence in corrected operator spectrum only some of nonrelativistic Hamiltonian eigenvalues not exceeding mentioned maximal possible kinetic energy value, i.e. $e_{nl} < mc^2/2$, are present. As a conclusion it follows that in infinite well finite number of solutions exists. Moreover, when radius of well stays smaller than some critical value, following from condition $\min e_{nl} \equiv e_{10} = mc^2/2$, spectrum of this operator is empty. For this radius definition one has to obtain minimal eigenvalue of corresponding well. Obviously, it will have angular momentum, that equal zero. Hence,

$$e_{10} = \frac{mc^2}{2} \left(\frac{\pi \hbar c}{Rmc^2} \right)^2. \quad (17)$$

Mentioned condition gives the following value of radius:

$$R = \frac{\pi \hbar c}{mc^2}. \quad (18)$$

Applying $\hbar c = 197.327 \text{ MeV fm}$ for proton ($mc^2 = 938.272 \text{ MeV}$) the radius of empty well equals $R_p = 0.660 \text{ fm}$. For electron ($mc^2 = 0.511 \text{ MeV}$) this radius is $R_e = 1.212 \text{ pm}$.

If the potential $v(\mathbf{r})$ does not equal identical zero, the Schrödinger equation is

$$(1 - 2\mathbf{T}_0/mc^2)^{-1} \mathbf{T}_0 \psi(\mathbf{r}) = (E - v(\mathbf{r})) \psi(\mathbf{r}). \quad (19)$$

Due to mentioned condition for operator $(1 - 2\mathbf{T}_0/mc^2)$ eigenvalues and obvious condition $(1 - 2\mathbf{T}_0/mc^2) \psi(\mathbf{r}) \neq 0$, this equation can be present in a following form:

$$\mathbf{T}_0 \psi(\mathbf{r}) = (1 - 2\mathbf{T}_0/mc^2) (E - v(\mathbf{r})) \psi(\mathbf{r}), \quad (20)$$

or

$$[1 - 2v(\mathbf{r}) + 2E] \mathbf{T}_0 \psi(\mathbf{r}) + mc^2 [v(\mathbf{r}) - E] \psi(\mathbf{r}) - 2[\mathbf{T}_0, v(\mathbf{r})] \psi(\mathbf{r}) = 0 \quad (21)$$

with aforementioned condition for corrected kinetic energy value

$$\int d\mathbf{r} \psi^+(\mathbf{r}) \mathbf{T}_0 \psi(\mathbf{r}) < mc^2/2. \quad (22)$$

The $[\mathbf{T}_0, v(\mathbf{r})]$ denotes commutator of nonrelativistic kinetic energy (8) and potential operators.

The equation obtained (21) is not trivial, its solutions, i.e. spectrum and eigenfunctions for different potentials, can give interesting information about relativistic effects in Schrödinger formalism at minimal relativity taken into account.

In conclusion one has to pay attention to the fact that factor $\gamma^2 = (1 - 2\mathbf{T}_0/mc^2)^{-1}$ appears in front of entire relativistic kinetic energy expression (3), hence the obtained results can be more fundamental than simple "kinematic relativity" approach.

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